CASINO Developed for Coupled Quantum Monte Carlo with Molecular Dynamics by HECToR dCSE Team

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HPC experts from UCL, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have successfully improved the capability of the CASINO quantum Monte Carlo code, by enabling scalable coupled calculations with the molecular dynamics code PWscf from the Quantum ESPRESSO package.

The CASINO code is a software package which is used to perform electronic structure calculations which are based on the quantum Monte Carlo (QMC) method. CASINO is very suitable for use on distributed HPC architectures due to the excellent scalability of the QMC method. CASINO is used regularly on HECToR with 10,000s cores or more and on international HPC resources. In particular, calculations involving 82,944 cores on the Jaguar Cray XT5 machine (1.75 petaFLOPS) at Oak Ridge National Laboratory, have been demonstrated.

Commenting on the dCSE project success, *Prof Dario Alfè of the Department of Physics and Astronomy at UCL said: "The DCSE development work has been very useful to CASINO. The main objective of the work was to implement the feature of coupled DFT-QMC molecular dynamics, which allows one to compute free energy differences between QMC and DFT in an efficient way. The implementation also removed several bottlenecks, including the generation of the trial wavefunctions in the DFT code PWSCF and their transformation into B-splines representations, which are now done in parallel and can therefore be several hundred times faster for big systems."*

For a fixed target of 100 per core for a total walker population, linear weak scalability has been demonstrated with 82,944 cores for a coupled DFT-QMC molecular dynamics simulation with CASINO version 2.7. This gives a dramatic reduction in simulation time and means it will be possible to use CASINO on machines with in excess of 100,000 cores.

"Since it is a specific new feature, it is difficult to predict how many users will use this implementation. We initially plan to use this to perform electronic structure calculations for water, and many more applications will follow in our group. I should also add that the two DCSE that we had the fortune to manage were instrumental in enabling access and large allocations on machines in the US, under the INCITE programme (over 400 million CPU hours, i.e. the equivalent of ~2 billion AU's on HECToR) in the 2010-2015 period. This would have not happened without the DCSE work."

HECToR

HECToR is managed by EPSRC on behalf of the participating Research Councils with a mission to support capability science and engineering in UK academia. The Cray XE6 supercomputer, located at the University of Edinburgh, is managed by UoE HPCx Ltd. The CSE Support Service is provided by NAG Ltd and ensures users have access to appropriate HPC expertise to effectively exploit advanced supercomputers for their science. A critical feature of the CSE Support Service is the distributed CSE (dCSE) programme which, through lightweight peer review, delivers dedicated performance and scalability projects on specific codes in response to proposals from users. The dCSE programme now consists of over 70 focused projects complementing the traditional HPC user applications support and training also provided by NAG.

The dCSE projects completed so far have delivered outstanding examples of the cost savings and new science that can be enabled through dedicated CSE effort. The CASINO project reported here adds to these success stories with a successful performance improvement.

Project Background

The objectives of this dCSE project were to develop CASINO to enable coupled Diffusion Monte Carlo (DMC) and Density Functional Theory (DFT) molecular dynamics simulations. This was achieved by modifications to CASINO with an algorithm that is based on re-weighting, level-cross checking and periodic Jastrow re-computation, together with an interface enabling the DFT and DMC data communication and transfer.

Prof Dario Alfè of the Department of Physics and Astronomy at UCL was the Principal Investigator for the project. Norbert Nemec and Mike Towler, also of UCL carried out the 18 person-month project, in close collaboration with the NAG CSE team.

Project Results

Firstly, an interface between PWscf and CASINO was developed. This is now provided through a file with a standard format containing: geometry, basis set, and orbital coefficients. Secondly, the parallel efficiency of the coupled DMC algorithm was optimised by improving the allocation and re-distribution of walkers (i.e. the list of current electron positions for the configuration, along with various associated quantities related to the energy and wave function) between the cores. This was achieved by implementing asynchronous communication to overlap with computation. Further minor modifications were also made to the CASINO distribution including the following: multiple pseudopotentials for elements with the same atomic number, support for running multiple jobs simultaneously, faster partial-ranking algorithm, interface support for CRYSTAL09 and a major revision of the user manual.

For a fixed target of 100 per core for a total walker population, linear weak scalability was demonstrated for over 80,000 cores on the Jaguar Cray XT5 machine (1.75 petaFLOPS) at Oak Ridge National Laboratory. Furthermore, with 82,944 cores, this new version of CASINO (2.7) is more than 30% faster than the previous one (2.6) and the total cost of re-distributing walkers (including the DMC equilibration) has reduced from 412 seconds to 1 second. This means it will be possible to use CASINO on machines with in excess of 100,000 cores.

A full technical report on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/casino02/

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